§8. Ab initio Molecular Dynamics Study of Graphite Erosion and Formation of Hydrocarbon Molecules by Absorption of Many Hydrogen Atoms

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The most important and urgent thing for achievement of magnetically confined nuclear fusion may be to find suitable wall materials of a fusion reactor having both heat and radiation resistances. Researches show that the wall surface is damaged not only by the physical sputtering process but also through chemical reactions (sputtering), the latter of which is confirmed to have major influences on the damaging of the fusion reactor wall.

As a typical example of the chemical sputtering, we study the erosion process of graphite by means of the *ab initio* (first-principle) molecular dynamics (MD) simulation code SIESTA [1]. In the code, the electron distributions in materials are determined by solving the Kohn-Sham equation, which is based on the density functional theory of quantum mechanics. We use parallel computers (PC cluster) each consisting of four Pentium 4/64-bits to handle massive computations [2].

Previously we found by *ab initio* MD that hydrocarbon molecules CH_n with n>1 are not formed on a flat (undamaged) graphite because of strong attraction between H and C atoms [3]. Experimentally, on the other hand, hydrocarbon molecules are generated through the chemical sputtering when graphite absorbs large number of hydrogen atoms. Being enlightened by this experiment, we have started a new series of *ab initio* MD simulations.

The simulated system is made of five carbon layers of graphen sheets. Hydrogen atoms are added to the space around the specific layer of the graphite, and they are naturally adsorbed by the layer. When the number of adsorbed hydrogen atoms per graphite layer reaches about 50% that of carbon atoms, the graphite layer is deformed to a highly non-flat shape (hills and valleys) and hydrocarbon molecules such as CH_2 and CH_3 are formed by cutting the covalent bonds between carbon atoms. This has become possible due to the stretching of the specific C-C bonds.

Incidentally, in experiments the amount of the hydrocarbon generation rate in the graphite increases at high temperature around 900K. We have shown by simulations that the already adsorbed hydrogen atoms are detached from the surface due to thermal vibrations at this temperature, thus the chemical sputtering is suppressed. Moreover, the CH_3 molecules already formed on the graphite layer at low temperatures are detached from the graphite layer at high temperature. We find that a big hole is created on the graphite layer after a CH_3 molecule has left, which facilitates further destruction of the layer.

As the applications of our research results, we propose to keep the wall material in high temperatures (around 1000K) to avoid its erosion by chemical sputtering. Also, a graphite-based material can be utilized as the hydrogen storage medium by controlling its temperature.

References

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[4] T. Koga and M. Tanaka, J. Korean Phys. Soc., in press (2006)

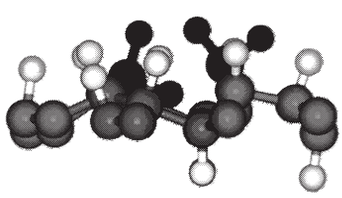

Fig.1 The molecular picture of the graphite layer after the absorption of many hydrogen atoms. White and gray balls denote hydrogen and carbon atoms, respectively, and a black molecule denotes CH_2.

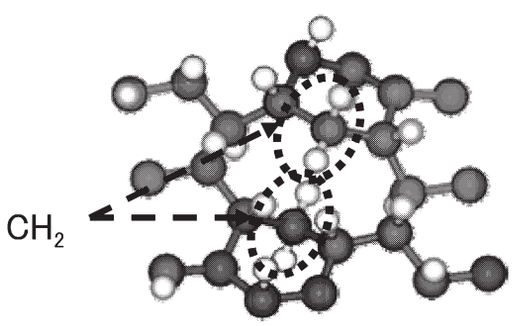

Fig.2 The eroded graphite with a created big hole after the formation of hydrocarbon molecules.